Random projection trees for vector quantization

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Abstract

A simple and computationally efficient scheme for tree-structured vector quantization is presented. Unlike previous methods, its quantization error depends only on the intrinsic dimension of the data distribution, rather than the apparent dimension of the space in which the data happen to lie.

1 Introduction

For a distribution P on $\mathbb{R}^D$, the *kth quantization error* is commonly defined as

$$\inf_{\mu_1,\ldots,\mu_k \in \mathbb{R}^D} \mathbb{E}\left[\min_{1\leq j\leq k} \|X-\mu_j\|^2\right],$$

where $\|\cdot\|$ denotes Euclidean norm and the expectation is over X drawn at random from P. It is known [15] that this infimum is realized, though perhaps not uniquely, by some set of points $\mu_1,\ldots,\mu_k$, called a *k-optimal set of centers*. The resulting quantization error has been shown to be roughly $k^{-2/D}$ under a variety of different assumptions on P [8]. This is discouraging when D is high. For instance, if $D = 1000$, it means that to merely halve the error, you need 2^{500} times as many codewords! In short, vector quantization is susceptible to the same *curse of dimensionality* that has been the bane of other nonparametric statistical methods.

A recent positive development in statistics and machine learning has been the realization that a lot of data that superficially lie in a high-dimensional space $\mathbb{R}^D$, actually have low *intrinsic* dimension, in the sense of lying close to a manifold of dimension $d \ll D$. We will give several examples of this below. There has thus been a huge interest in algorithms that *learn* this manifold from data, with the intention that future data can then be transformed into this low-dimensional space, in which the usual nonparametric (and other) methods will work well [18, 16, 2].

In this paper, we are interested in techniques that automatically adapt to intrinsic low dimensional structure without having to explicitly learn this structure. We describe a tree-structured vector quantizer whose quantization error is $k^{-1/O(d)}$; that is to say, its error rate depends only on the low intrinsic dimension rather than the high apparent dimension. The quantizer is based on a hierarchical decomposition of $\mathbb{R}^D$: first the entire space is split into two pieces, then each of these pieces is further split in two, and so on, until a partition of k cells is reached. Each codeword is the mean of the distribution restricted to one of these cells.

Tree-structured vector quantizers abound; the power of our approach comes from the particular splitting method. To divide a region S into two, we pick a random direction from the surface of the unit sphere in $\mathbb{R}^D$, and split S at the median of its projection onto this direction (Figure 1). We call the resulting spatial partition a *random projection tree* or *RP tree*.

At first glance, it might seem that a better way to split a region is to find the 2-optimal set of centers for it. However, as we explain below, this is an NP-hard optimization problem, and is therefore unlikely to be computationally tractable. Although there are several algorithms that attempt to solve this problem, such as Lloyd's method [12, 11], they are not in general able to find the optimal solution. In fact, they are often far from optimal.

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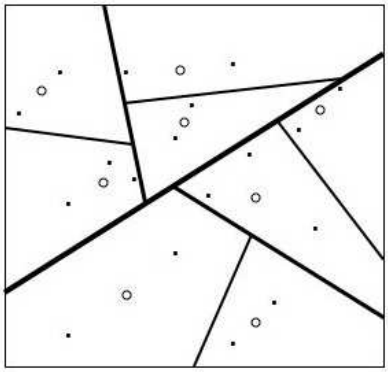

Figure 1: Spatial partitioning of $\mathbb{R}^2$ induced by an RP tree with three levels. The dots are data points; each circle represents the mean of the vectors in one cell.

For our random projection trees, we show that if the data have intrinsic dimension d (in a sense we make precise below), then each split pares off about a $1/d$ fraction of the quantization error. Thus, after $\log k$ levels of splitting, there are k cells and the quantization error is of the form $(1 - 1/d)^{\log k} = k^{-1/O(d)}$. There is no dependence at all on the extrinsic dimensionality D.

2 Detailed overview

2.1 Low-dimensional manifolds

The increasing ubiquity of massive, high-dimensional data sets has focused the attention of the statistics and machine learning communities on the curse of dimensionality. A large part of this effort is based on exploiting the observation that many high-dimensional data sets have low *intrinsic dimension*. This is a loosely defined notion, which is typically used to mean that the data lie near a smooth low-dimensional manifold.

For instance, suppose that you wish to create realistic animations by collecting human motion data and then fitting models to it. A common method for collecting motion data is to have a person wear a skin-tight suit with high contrast reference points printed on it. Video cameras are used to track the 3D trajectories of the reference points as the person is walking or running. In order to ensure good coverage, a typical suit has about $N = 100$ reference points. The position and posture of the body at a particular point of time is represented by a $(3N)$-dimensional vector. However, despite this seeming high dimensionality, the number of degrees of freedom is small, corresponding to the dozen-or-so joint angles in the body. The positions of the reference points are more or less deterministic functions of these joint angles.

Interestingly, in this example the intrinsic dimension becomes even smaller if we *double* the dimension of the embedding space by including for each sensor its relative velocity vector. In this space of dimension $6N$ the measured points will lie very close to the *one* dimensional manifold describing the combinations of locations and speeds that the limbs go through during walking or running.

To take another example, a speech signal is commonly represented by a high-dimensional time series: the signal is broken into overlapping windows, and a variety of filters are applied within each window. Even richer representations can be obtained by using more filters, or by concatenating vectors corresponding to consecutive windows. Through all this, the intrinsic dimensionality remains small, because the system can be described by a few physical parameters describing the configuration of the speaker's vocal apparatus.

In machine learning and statistics, almost all the work on exploiting intrinsic low dimensionality consists of algorithms for learning the structure of these manifolds; or more precisely, for learning embeddings of these manifolds into low-dimensional Euclidean space. Our contribution is a simple and compact data structure that automatically exploits the low intrinsic dimensionality of data on a local level without having to explicitly learn the global manifold structure.

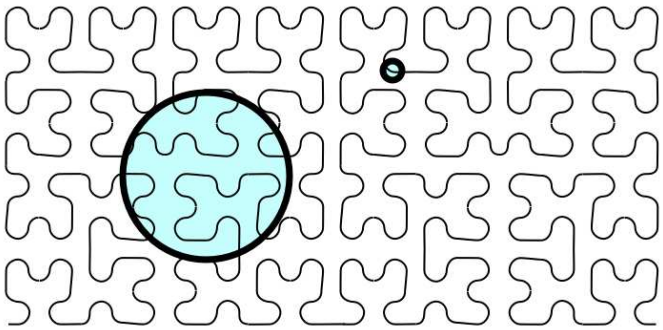

Figure 2: Hilbert's space filling curve. Large neighborhoods look 2-dimensional, smaller neighborhoods look 1-dimensional, and even smaller neighborhoods would consist mostly of measurement noise and would therefore again be 2-dimensional.

2.2 Defining intrinsic dimensionality

Low-dimensional manifolds are our inspiration and source of intuition, but when it comes to precisely defining intrinsic dimension for data analysis, the differential geometry concept of manifold is not entirely suitable. First of all, any data set lies on a one-dimensional manifold, as evidenced by the construction of space-filling curves. Therefore, some bound on curvature is implicitly needed. Second, and more important, it is unreasonable to expect data to lie *exactly* on a low-dimensional manifold. At a certain small resolution, measurement error and noise make any data set full-dimensional. The most we can hope is that the data distribution is concentrated *near* a low-dimensional manifold of bounded curvature (Figure 2).

We address these various concerns with a statistically-motivated notion of dimension: we say that a set S has *local covariance dimension* (d, ϵ, r) if neighborhoods of radius r have $(1-\epsilon)$ fraction of their variance concentrated in a d-dimensional subspace. To make this precise, start by letting $\sigma_1^2, \sigma_2^2, \ldots, \sigma_D^2$ denote the eigenvalues of the covariance matrix; these are the variances in each of the eigenvector directions.

Definition 1 *Set $S \subset \mathbb{R}^D$ has local covariance dimension (d, ϵ, r) if its restriction to any ball of radius r has covariance matrix whose largest d eigenvalues satisfy*

$$\sigma_1^2 + \cdots + \sigma_d^2 \;\geq\; (1-\epsilon) \cdot (\sigma_1^2 + \cdots + \sigma_D^2).$$

2.3 Random projection trees

Our new data structure, the random projection tree, is built by recursive binary splits. The core tree-building algorithm is called MAKETREE, which takes as input a data set $S \subset \mathbb{R}^D$, and repeatedly calls a splitting subroutine CHOOSERULE.

procedure MAKETREE(S)
 if $|S| < MinSize$ **then return** $(Leaf)$
 $Rule \leftarrow$ CHOOSERULE(S)
 $LeftTree \leftarrow$ MAKETREE($\{x \in S : Rule(x) = \text{true}\}$)
 $RightTree \leftarrow$ MAKETREE($\{x \in S : Rule(x) = \text{false}\}$)
 return $([Rule, LeftTree, RightTree])$

The RP tree has two types of split. Typically, a direction is chosen uniformly at random from surface of the unit sphere and the cell is split at its median, by a hyperplane orthogonal to this direction. Occasionally, a different type of split is used, in which a cell is split into two pieces based on distance from the mean.

procedure CHOOSERULE(S)
 if $\Delta^2(S) \leq c \cdot \Delta_A^2(S)$
  then $\begin{cases} \text{choose a random unit direction } v \\ Rule(x) := x \cdot v \leq \text{median}(\{z \cdot v : z \in S\}) \end{cases}$
  else $\begin{cases} Rule(x) := \\ \|x - \text{mean}(S)\| \leq \text{median}(\{\|z - \text{mean}(S)\| : z \in S\}) \end{cases}$
 return $(Rule)$

In the code, c is a constant, $\Delta(S)$ is the diameter of S (the distance between the two furthest points in the set), and $\Delta_A(S)$ is the *average* diameter, that is, the average distance between points of S:

$$\Delta_A^2(S) = \frac{1}{|S|^2} \sum_{x,y \in S} \|x - y\|^2.$$

2.4 Main result

Suppose an RP tree is built from a data set $S \subset \mathbb{R}^D$, not necessarily finite. If the tree has k levels, then it partitions the space into 2^k cells. We define the *radius* of a cell $C \subset \mathbb{R}^D$ to be the smallest $r > 0$ such that $S \cap C \subset B(x, r)$ for some $x \in C$.

Recall that an RP tree has two different types of split; let's call them splits *by distance* and splits *by projection*.

Theorem 2 *There are constants $0 < c_1, c_2, c_3 < 1$ with the following property. Suppose an RP tree is built using data set $S \subset \mathbb{R}^D$. Consider any cell C of radius r, such that $S \cap C$ has local covariance dimension (d, ϵ, r), where $\epsilon < c_1$. Pick a point $x \in S \cap C$ at random, and let C' be the cell that contains it at the next level down.*

- *If C is split by distance, $\mathbb{E}\left[\Delta(S \cap C')\right] \leq c_2 \Delta(S \cap C)$.*
- *If C is split by projection, then $\mathbb{E}\left[\Delta_A^2(S \cap C')\right] \leq (1 - (c_3/d))\, \Delta_A^2(S \cap C)$.*

In both cases, the expectation is over the randomization in splitting C and the choice of $x \in S \cap C$.

2.5 The hardness of finding optimal centers

Given a data set, the optimization problem of finding a k-optimal set of centers is called the k-means problem. Here is the formal definition.

> k-MEANS CLUSTERING
>
> *Input:* Set of points $x_1, \ldots, x_n \in \mathbb{R}^D$; integer k.
>
> *Output:* A partition of the points into clusters $C_1, \ldots, C_k$, along with a center μ_j for each cluster, so as to minimize
>
> $$\sum_{j=1}^{k} \sum_{i \in C_j} \|x_i - \mu_j\|^2.$$

The typical method of approaching this task is to apply Lloyd's algorithm [12, 11], and usually this algorithm is itself called k-means. The distinction between the two is particularly important to make because Lloyd's algorithm is a heuristic that often returns a suboptimal solution to the k-means problem. Indeed, its solution is often very far from optimal.

What's worse, this suboptimality is not just a problem with Lloyd's algorithm, but an inherent difficulty in the optimization task. k-MEANS CLUSTERING is an NP-hard optimization problem, which means that it is very unlikely that there exists an efficient algorithm for it. To explain this a bit more clearly, we delve briefly into the theory of computational complexity.

The running time of an algorithm is typically measured as a function of its input/output size. In the case of k-means, for instance, it would be given as a function of n, k, and D. An efficient algorithm is one whose running time

scales *polynomially* with the problem size. For instance, there are algorithms for sorting n numbers which take time proportional to $n \log n$; these qualify as efficient because $n \log n$ is bounded above by a polynomial in n.

For some optimization problems, the best algorithms we know take time *exponential* in problem size. The famous traveling salesman problem (given distances between n cities, plan a circular route through them so that each city is visited once and the overall tour length is minimized) is one of these. There are various algorithms for it that take time proportional to 2^n (or worse): this means each additional city causes the running time to be doubled! Even small graphs are therefore hard to solve.

This disturbing lack of an efficient algorithm is not limited to just a few pathological optimization tasks. Rather, it is an epidemic across the entire spectrum of computational tasks, one that afflicts thousands of the problems we most urgently want to solve. Amazingly, it has been shown that the fates of these diverse problems (called *NP-complete* problems) are linked: either *all* of them admit efficient algorithms, or none of them do! The mathematical community strongly believes the latter to be the case, although it is has not been proved. Resolving this question is one of the seven "grand challenges" of the new millenium identified by the Clay Institute.

In Appendix II, we show the following.

Theorem 3 k-MEANS CLUSTERING *is an NP-hard optimization problem, even if* k *is restricted to 2.*

Thus we cannot expect to be able to find a k-optimal set of centers; the best we can hope is to find some set of centers that achieves roughly the optimal quantization error.

2.6 Related work

Quantization

The literature on vector quantization is substantial; see the wonderful survey of Gray and Neuhoff [9] for a comprehensive overview. In the most basic setup, there is some distribution P over $\mathbb{R}^D$ from which random vectors are generated and observed, and the goal is to pick a finite codebook $C \subset \mathbb{R}^D$ and an encoding function $\alpha : \mathbb{R}^D \to C$ such that $x \approx \alpha(x)$ for typical vectors x. The quantization error is usually measured by squared loss, $\mathbb{E}\|X - \alpha(X)\|^2$. An obvious choice is to let $\alpha(x)$ be the nearest neighbor of x in C. However, the number of codewords is often so enormous that this nearest neighbor computation cannot be performed in real time. A more efficient scheme is to have the codewords arranged in a tree [4].

The asymptotic behavior of quantization error, assuming optimal quantizers and under various conditions on P, has been studied in great detail. A nice overview is presented in the recent monograph of Graf and Luschgy [8]. The rates obtained for k-optimal quantizers are generally of the form $k^{-2/D}$. There is also work on the special case of data that lie *exactly* on a manifold, and whose distribution is within some constant factor of uniform; in such cases, rates of the form $k^{-2/d}$ are obtained, where d is the dimension of the manifold. Our setting is considerably more general than this: we do not assume optimal quantization (which is NP-hard), we have a broad notion of intrinsic dimension that allows points to merely be close to a manifold rather than on it, and we make no other assumptions about the distribution P.

Compressed sensing

The field of compressed sensing has grown out of the surprising realization that high-dimensional sparse data can be accurately reconstructed from just a few random projections [3, 5]. The central premise of this research area is that the original data thus never even needs to be collected: all one ever sees are the random projections.

RP trees are similar in spirit and entirely compatible with this viewpoint. Theorem 2 holds even if the random projections are forced to be the same across each entire level of the tree. For a tree of depth k, this means only k random projections are ever needed, and these can be computed beforehand (the split-by-distance can be reworked to operate in the projected space rather than the high-dimensional space). The data are not accessed in any other way.

3 An RP tree adapts to intrinsic dimension

An RP tree has two varieties of split. If a cell C has much larger diameter than average-diameter (average interpoint distance), then it is split according to the distances of points from the mean. Otherwise, a random projection is used.

The first type of split is particularly easy to analyze.

3.1 Splitting by distance from the mean

This option is invoked when the points in the current cell, call them S, satisfy $\Delta^2(S) > c\Delta_A^2(S)$; recall that $\Delta(S)$ is the diameter of S while $\Delta_A^2(S)$ is the average interpoint distance.

Lemma 4 *Suppose that $\Delta^2(S) > c\Delta_A^2(S)$. Let S_1 denote the points in S whose distance to* mean(S) *is less than or equal to the median distance, and let S_2 be the remaining points. Then the expected squared diameter after the split is*

$$\frac{|S_1|}{|S|}\Delta^2(S_1) + \frac{|S_2|}{|S|}\Delta^2(S_2) \;\leq\; \left(\frac{1}{2} + \frac{2}{c}\right)\Delta^2(S).$$

The proof of this lemma is deferred to the Appendix, as are most of the other proofs in this paper.

3.2 Splitting by projection: proof outline

Suppose the current cell contains a set of points $S \subset \mathbb{R}^D$ for which $\Delta^2(S) \leq c\Delta_A^2(S)$. We will show that a split by projection has a constant probability of reducing the average squared diameter $\Delta_A^2(S)$ by $\Omega(\Delta_A^2(S)/d)$. Our proof has three parts:

I. Suppose S is split into S_1 and S_2, with means μ_1 and μ_2. Then the reduction in average diameter can be expressed in a remarkably simple form, as a multiple of $\|\mu_1 - \mu_2\|^2$.

II. Next, we give a lower bound on the distance between the *projected* means, $(\widetilde{\mu}_1 - \widetilde{\mu}_2)^2$. We show that the distribution of the projected points is subgaussian with variance $O(\Delta_A^2(S)/D)$. This well-behavedness implies that $(\widetilde{\mu}_1 - \widetilde{\mu}_2)^2 = \Omega(\Delta_A^2(S)/D)$.

III. We finish by showing that, approximately, $\|\mu_1 - \mu_2\|^2 \geq (D/d)(\widetilde{\mu}_1 - \widetilde{\mu}_2)^2$. This is because $\mu_1 - \mu_2$ lies close to the subspace spanned by the top d eigenvectors of the covariance matrix of S; and with high probability, *every* vector in this subspace shrinks by $O(\sqrt{d/D})$ when projected on a random line.

We now tackle these three parts of the proof in order.

3.3 Quantifying the reduction in average diameter

The average squared diameter $\Delta_A^2(S)$ has certain reformulations that make it convenient to work with. These properties are consequences of the following two observations, the first of which the reader may recognize as a standard "bias-variance" decomposition of statistics.

Lemma 5 *Let X, Y be independent and identically distributed random variables in $\mathbb{R}^n$, and let $z \in \mathbb{R}^n$ be any fixed vector.*

(a) $\mathbb{E}\left[\|X - z\|^2\right] = \mathbb{E}\left[\|X - \mathbb{E}X\|^2\right] + \|z - \mathbb{E}X\|^2$.

(b) $\mathbb{E}\left[\|X - Y\|^2\right] = 2\,\mathbb{E}\left[\|X - \mathbb{E}X\|^2\right]$.

Proof. Part (a) is immediate when both sides are expanded. For (b), we use part (a) to assert that for any fixed y, we have $\mathbb{E}\left[\|X - y\|^2\right] = \mathbb{E}\left[\|X - \mathbb{E}X\|^2\right] + \|y - \mathbb{E}X\|^2$. We then take expectation over $Y = y$. ∎

This can be used to show that the averaged squared diameter, $\Delta_A^2(S)$, is twice the average squared distance of points in S from their mean.

Corollary 6 *The average squared diameter of a set S can also be written as:*

$$\Delta_A^2(S) = \frac{2}{|S|}\sum_{x\in S}\|x - \text{mean}(S)\|^2.$$

Proof. $\Delta_A^2(S)$ is simply $\mathbb{E}\left[\|X-Y\|^2\right]$, when X, Y are i.i.d. draws from the uniform distribution over S. ∎

At each successive level of the tree, the current cell is split into two, either by a random projection or according to distance from the mean. Suppose the points in the current cell are S, and that they are split into sets S_1 and S_2. It is obvious that the expected diameter is nonincreasing:

$$\Delta(S) \;\geq\; \frac{|S_1|}{|S|}\Delta(S_1) + \frac{|S_2|}{|S|}\Delta(S_2).$$

This is also true of the expected average diameter. In fact, we can precisely characterize how much it decreases on account of the split.

Lemma 7 *Suppose set S is partitioned (in any manner) into S_1 and S_2. Then*

$$\Delta_A^2(S) - \left\{\frac{|S_1|}{|S|}\Delta_A^2(S_1) + \frac{|S_2|}{|S|}\Delta_A^2(S_2)\right\} \;=\; \frac{2|S_1|\cdot|S_2|}{|S|^2}\|\text{mean}(S_1) - \text{mean}(S_2)\|^2.$$

This completes part I of the proof outline.

3.4 Properties of random projections

Our quantization scheme depends heavily upon certain regularity properties of random projections. We now review these properties, which are critical for parts II and III of our proof.

The most obvious way to pick a random projection from $\mathbb{R}^D$ to $\mathbb{R}$ is to choose a projection direction u uniformly at random from the surface of the unit sphere S^{D-1}, and to send $x \mapsto u \cdot x$.

Another common option is to select the projection vector from a multivariate Gaussian distribution, $u \sim N(0, (1/D)I_D)$. This gives almost the same distribution as before, and is slightly easier to work with in terms of the algorithm and analysis. We will therefore use this type of projection, bearing in mind that all proofs carry over to the other variety as well, with slight changes in constants.

The key property of a random projection from $\mathbb{R}^D$ to $\mathbb{R}$ is that it approximately preserves the lengths of vectors, modulo a scaling factor of $\sqrt{D}$. This is summarized in the lemma below.

Lemma 8 *Fix any $x \in \mathbb{R}^D$. Pick a random vector $U \sim N(0, (1/D)I_D)$. Then for any $\alpha, \beta > 0$:*

(a) $\mathbb{P}\left[|U\cdot x| \leq \alpha\cdot\frac{\|x\|}{\sqrt{D}}\right] \;\leq\; \sqrt{\frac{2}{\pi}}\,\alpha$

(b) $\mathbb{P}\left[|U\cdot x| \geq \beta\cdot\frac{\|x\|}{\sqrt{D}}\right] \;\leq\; \frac{2}{\beta}e^{-\beta^2/2}$

Lemma 8 applies to any individual vector. Thus it also applies, in expectation, to a vector chosen at random from a set $S \subset \mathbb{R}^D$. Applying Markov's inequality, we can then conclude that when S is projected onto a random direction, *most* of the projected points will be close together, in a *central interval* of size $O(\Delta(S)/\sqrt{D})$.

Lemma 9 *Suppose $S \subset \mathbb{R}^D$ lies within some ball $B(x_0, \Delta)$. Pick any $0 < \delta, \epsilon \leq 1$ such that $\delta\epsilon \leq 1/e^2$. Let ν be any measure on S. Then with probability $> 1-\delta$ over the choice of random projection U onto $\mathbb{R}$, all but an ϵ fraction of $U\cdot S$ (measured according to ν) lies within distance $\sqrt{2\ln\frac{1}{\delta\epsilon}}\cdot\frac{\Delta}{\sqrt{D}}$ of $U\cdot x_0$.*

As a corollary, the median of the projected points must also lie within this central interval.

Corollary 10 *Under the hypotheses of Lemma 9, for any $0 < \delta < 2/e^2$, the following holds with probability at least $1 - \delta$ over the choice of projection:*

$$|\text{median}(U \cdot S) - U \cdot x_0| \;\leq\; \frac{\Delta}{\sqrt{D}} \cdot \sqrt{2 \ln \frac{2}{\delta}}.$$

Proof. Let ν be the uniform distribution over S and use $\epsilon = 1/2$. ∎

Finally, we examine what happens when the set S is a d-dimensional subspace of $\mathbb{R}^D$. Lemma 8 tells us that the projection of any *specific* vector $x \in S$ is unlikely to have length too much greater than $\|x\|/\sqrt{D}$, with high probability. A slightly weaker bound can be shown to hold for all of S simultaneously; the proof technique has appeared before in several contexts, including [14, 1].

Lemma 11 *There exists a constant κ_1 with the following property. Fix any $\delta > 0$ and any d-dimensional subspace $H \subset \mathbb{R}^D$. Pick a random projection $U \sim N(0, (1/D)I_D)$. Then with probability at least $1 - \delta$ over the choice of U,*

$$\sup_{x \in H} \frac{|x \cdot U|^2}{\|x\|^2} \;\leq\; \kappa_1 \cdot \frac{d + \ln 1/\delta}{D}.$$

Proof. It is enough to show that the inequality holds for $S = H \cap$ (surface of the unit sphere in $\mathbb{R}^D$). Let N be any $(1/2)$-cover of this set; it is possible to achieve $|N| \leq 10^d$ [13]. Apply Lemma 8, along with a union bound, to conclude that with probability at least $1 - \delta$ over the choice of projection U,

$$\sup_{x \in N} |x \cdot U|^2 \;\leq\; 2 \cdot \frac{\ln |N| + \ln 1/\delta}{D}.$$

Now, define C by

$$C \;=\; \sup_{x \in S} \left(|x \cdot U|^2 \cdot \frac{D}{\ln |N| + \ln 1/\delta} \right).$$

We'll complete the proof by showing $C \leq 8$. To this end, pick the $x^* \in S$ for which the supremum is realized (note S is compact), and choose $y \in N$ whose distance to x^* is at most $1/2$. Then,

$$\begin{aligned} |x^* \cdot U| &\leq |y \cdot U| + |(x^* - y) \cdot U| \\ &\leq \sqrt{\frac{\ln |N| + \ln 1/\delta}{D}} \left(\sqrt{2} + \frac{1}{2}\sqrt{C} \right) \end{aligned}$$

From the definition of x^*, it follows that $\sqrt{C} \leq \sqrt{2} + \sqrt{C}/2$ and thus $C \leq 8$. ∎

3.5 Properties of the projected data

Projection from $\mathbb{R}^D$ into $\mathbb{R}^1$ shrinks the average squared diameter of a data set by roughly D. To see this, we start with the fact that when a data set with covariance A is projected onto a vector U, the projected data have variance $U^T A U$. We now show that for random U, such quadratic forms are concentrated about their expected values.

Lemma 12 *Suppose A is an $n \times n$ positive semidefinite matrix, and $U \sim N(0, (1/n)I_n)$. Then for any $\alpha, \beta > 0$:*

(a) $\mathbb{P}[U^T A U < \alpha \cdot \mathbb{E}[U^T A U]] \leq e^{-((1/2)-\alpha)/2}$, *and*

(b) $\mathbb{P}[U^T A U > \beta \cdot \mathbb{E}[U^T A U]] \leq e^{-(\beta-2)/4}$.

Lemma 13 *Pick $U \sim N(0,(1/D)I_D)$. Then for any $S \subset \mathbb{R}^D$, with probability at least $1/10$, the projection of S onto U has average squared diameter*

$$\Delta_A^2(S \cdot U) \geq \frac{\Delta_A^2(S)}{4D}.$$

Proof. By Corollary 6,

$$\Delta_A^2(S \cdot U) \;=\; \frac{2}{|S|}\sum_{x \in S}((x - \text{mean}(S)) \cdot U)^2 \;=\; 2U^T \text{cov}(S) U.$$

where $\text{cov}(S)$ is the covariance of data set S. This quadratic term has expectation (over choice of U)

$$\begin{aligned}\mathbb{E}[2U^T\text{cov}(S)U] &= 2\sum_{i,j}\mathbb{E}[U_iU_j]\text{cov}(S)_{ij} \\ &= \frac{2}{D}\sum_i \text{cov}(S)_{ii} \;=\; \frac{\Delta_A^2(S)}{D}.\end{aligned}$$

Lemma 12(a) then bounds the probability that it is much smaller than its expected value. ∎

Next, we examine the overall distribution of the projected points. When $S \subset \mathbb{R}^D$ has diameter Δ, its projection into the line can have diameter upto Δ, but as we saw in Lemma 9, most of it will lie within a central interval of size $O(\Delta/\sqrt{D})$. What can be said about points that fall outside this interval?

Lemma 14 *Suppose $S \subset B(0,\Delta) \subset \mathbb{R}^D$. Pick any $\delta > 0$ and choose $U \sim N(0,(1/D)I_D)$. Then with probability at least $1-\delta$ over the choice of U, the projection $S \cdot U = \{x \cdot U : x \in S\}$ satisfies the following property for all positive integers k.*

The fraction of points outside the interval $\left(-\frac{k\Delta}{\sqrt{D}}, +\frac{k\Delta}{\sqrt{D}}\right)$ is at most $\frac{2^k}{\delta} \cdot e^{-k^2/2}$.

Proof. This follows by applying Lemma 9 for each positive integer k (with corresponding failure probability $\delta/2^k$), and then taking a union bound. ∎

3.6 Distance between the projected means

We are dealing with the case when $\Delta^2(S) \leq c \cdot \Delta_A^2(S)$, that is, the diameter of set S is at most a constant factor times the average interpoint distance. If S is projected onto a random direction, the projected points will have variance about $\Delta_A^2(S)/D$, by Lemma 13; and by Lemma 14, it isn't too far from the truth to think of these points as having roughly a Gaussian distribution. Thus, if the projected points are split into two groups at the mean, we would expect the means of these two groups to be separated by a distance of about $\Delta_A(S)/\sqrt{D}$. Indeed, this is the case. The same holds if we split at the median, which isn't all that different from the mean for close-to-Gaussian distributions.

Lemma 15 *There is a constant κ_2 for which the following holds. Pick any $0 < \delta < 1/16c$. Pick $U \sim N(0,(1/D)I_D)$ and split S into two pieces:*

$$S_1 = \{x \in S : x \cdot U < s\} \;\; \textit{and} \;\; S_2 = \{x \in S : x \cdot U \geq s\},$$

where s is either $\text{mean}(S \cdot U)$ *or median$(S \cdot U)$. Write $p = |S_1|/|S|$, and let $\widetilde{\mu}_1$ and $\widetilde{\mu}_2$ denote the means of $S_1 \cdot U$ and $S_2 \cdot U$, respectively. Then with probability at least $1/10 - \delta$,*

$$(\widetilde{\mu}_2 - \widetilde{\mu}_1)^2 \;\geq\; \kappa_2 \cdot \frac{1}{(p(1-p))^2} \cdot \frac{\Delta_A^2(S)}{D} \cdot \frac{1}{c\,\log(1/\delta)}.$$

Proof. Let the random variable $\widetilde{X}$ denote a uniform-random draw from the projected points $S \cdot U$. Without loss of generality mean$(S) = 0$, so that $\mathbb{E}\widetilde{X} = 0$ and thus $p\widetilde{\mu}_1 + (1-p)\widetilde{\mu}_2 = 0$. Rearranging, we get $\widetilde{\mu}_1 = -(1-p)(\widetilde{\mu}_2 - \widetilde{\mu}_1)$ and $\widetilde{\mu}_2 = p(\widetilde{\mu}_2 - \widetilde{\mu}_1)$.

We already know from Lemma 13 (and Corollary 6) that with probability at least $1/10$, the variance of the projected points is significant: var$(\widetilde{X}) \geq \Delta_A^2(S)/8D$. We'll show this implies a similar lower bound on $(\widetilde{\mu}_2 - \widetilde{\mu}_1)^2$.

Using $\mathbf{1}(\cdot)$ to denote $0-1$ indicator variables,

$$\begin{aligned} \text{var}(\widetilde{X}) &\leq \mathbb{E}[(\widetilde{X} - s)^2] \\ &\leq \mathbb{E}[2t|\widetilde{X} - s| + (|\widetilde{X} - s| - t)^2 \cdot \mathbf{1}(|\widetilde{X} - s| \geq t)] \end{aligned}$$

for any $t > 0$. This is a convenient formulation since the linear term gives us $\widetilde{\mu}_2 - \widetilde{\mu}_1$:

$$\begin{aligned} \mathbb{E}[2t|\widetilde{X} - s|] &= 2t(p(s - \widetilde{\mu}_1) + (1-p)(\widetilde{\mu}_2 - s)) \\ &= 4t \cdot p(1-p) \cdot (\widetilde{\mu}_2 - \widetilde{\mu}_1) + 2ts(2p-1). \end{aligned}$$

The last term vanishes since the split is either at the mean of the projected points, in which case $s = 0$, or at the median, in which case $p = 1/2$.

Next, we'll choose

$$t = t_o \frac{\Delta(S)}{\sqrt{D}} \cdot \sqrt{\log \frac{1}{\delta}}$$

for some suitable constant t_o, so that the quadratic term in var$(\widetilde{X})$ can be bounded using Lemma 14 and Corollary 10: with probability at least $1 - \delta$,

$$E[(|\widetilde{X}| - t)^2 \cdot \mathbf{1}(|\widetilde{X}| \geq t)] \leq \delta \cdot \frac{\Delta^2(S)}{D}$$

(this is a simple integration). Putting the pieces together, we have

$$\frac{\Delta_A^2(S)}{8D} \leq \text{var}(\widetilde{X}) \leq 4t \cdot p(1-p) \cdot (\widetilde{\mu}_2 - \widetilde{\mu}_1) + \delta \cdot \frac{\Delta^2(S)}{D}.$$

The result now follows immediately by algebraic manipulation, using the relation $\Delta^2(S) \leq c\Delta_A^2(S)$. ∎

3.7 Distance between the high-dimensional means

Split S into two pieces as in the setting of Lemma 15, and let μ_1 and μ_2 denote the means of S_1 and S_2, respectively. We already have a lower bound on the distance between the projected means, $\widetilde{\mu}_2 - \widetilde{\mu}_1$; we will now show that $\|\mu_2 - \mu_1\|$ is larger than this by a factor of about $\sqrt{D/d}$. The main technical difficulty here is the dependence between the μ_i and the projection U. Incidentally, this is the only part of the entire argument that exploits intrinsic dimensionality.

Lemma 16 *There exists a constant κ_3 with the following property. Suppose set $S \subset \mathbb{R}^D$ is such that the top d eigenvalues of* cov(S) *account for more than $1 - \epsilon$ of its trace. Pick a random vector $U \sim N(0, (1/D)I_D)$, and split S into two pieces, S_1 and S_2, in any fashion (which may depend upon U). Let $p = |S_1|/|S|$. Let μ_1 and μ_2 be the means of S_1 and S_2, and let $\widetilde{\mu}_1$ and $\widetilde{\mu}_2$ be the means of $S_1 \cdot U$ and $S_2 \cdot U$.*

Then, for any $\delta > 0$, with probability at least $1 - \delta$ over the choice of U,

$$\|\mu_2 - \mu_1\|^2 \geq \frac{\kappa_3 D}{d + \ln 1/\delta} \left((\widetilde{\mu}_2 - \widetilde{\mu}_1)^2 - \frac{4}{p(1-p)} \frac{\epsilon \Delta_A^2(S)}{\delta D} \right).$$

Proof. Assume without loss of generality that S has zero mean. Let H denote the subspace spanned by the top d eigenvectors of the covariance matrix of S, and let $H^\perp$ be its orthogonal subspace. Write any point $x \in \mathbb{R}^D$ as $x_H + x_\perp$, where each component is seen as a vector in $\mathbb{R}^D$ that lies in the respective subspace.

Pick the random vector U; with probability $\geq 1 - \delta$ it satisfies the following two properties.

Property 1: For some constant $\kappa' > 0$, for every $x \in \mathbb{R}^D$

$$|x_H \cdot U|^2 \;\le\; \|x_H\|^2 \cdot \kappa' \cdot \frac{d + \ln 1/\delta}{D} \;\le\; \|x\|^2 \cdot \kappa' \cdot \frac{d + \ln 1/\delta}{D}.$$

This holds (with probability $1 - \delta/2$) by Lemma 11.
Property 2: Letting X denote a uniform-random draw from S, we have

$$\begin{aligned}
\mathbb{E}_X[(X_\perp \cdot U)^2] &\le \frac{2}{\delta} \cdot \mathbb{E}_U \mathbb{E}_X[(X_\perp \cdot U)^2] \\
&= \frac{2}{\delta} \cdot \mathbb{E}_X \mathbb{E}_U[(X_\perp \cdot U)^2] \\
&= \frac{2}{\delta D} \cdot \mathbb{E}_X[\|X_\perp\|^2] \;\le\; \frac{\epsilon \Delta_A^2(S)}{\delta D}.
\end{aligned}$$

The first step is Markov's inequality, and holds with probability $1 - \delta/2$. The last inequality comes from the local covariance condition.

So assume the two properties hold. Writing $\mu_2 - \mu_1$ as $(\mu_{2H} - \mu_{1H}) + (\mu_{2\perp} - \mu_{1\perp})$,

$$\begin{aligned}
(\widetilde{\mu}_2 - \widetilde{\mu}_1)^2 &= ((\mu_{2H} - \mu_{1H}) \cdot U + (\mu_{2\perp} - \mu_{1\perp}) \cdot U)^2 \\
&\le 2((\mu_{2H} - \mu_{1H}) \cdot U)^2 + 2((\mu_{2\perp} - \mu_{1\perp}) \cdot U)^2.
\end{aligned}$$

The first term can be bounded by Property 1:

$$((\mu_{2H} - \mu_{1H}) \cdot U)^2 \;\le\; \|\mu_2 - \mu_1\|^2 \cdot \kappa' \cdot \frac{d + \ln 1/\delta}{D}.$$

For the second term, let $\mathbb{E}_X$ denote expectation over X chosen uniformly at random from S. Then

$$\begin{aligned}
((\mu_{2\perp} - \mu_{1\perp}) \cdot U)^2 &\le 2(\mu_{2\perp} \cdot U)^2 + 2(\mu_{1\perp} \cdot U)^2 \\
&= 2(\mathbb{E}_X[X_\perp \cdot U \mid X \in S_2])^2 + 2(\mathbb{E}_X[X_\perp \cdot U \mid X \in S_1])^2 \\
&\le 2\mathbb{E}_X[(X_\perp \cdot U)^2 \mid X \in S_2] + 2\mathbb{E}_X[(X_\perp \cdot U)^2 \mid X \in S_1] \\
&\le \frac{2}{1-p} \cdot \mathbb{E}_X[(X_\perp \cdot U)^2] + \frac{2}{p} \cdot \mathbb{E}_X[(X_\perp \cdot U)^2] \\
&= \frac{2}{p(1-p)} \mathbb{E}_X[(X_\perp \cdot U)^2] \;\le\; \frac{2}{p(1-p)} \cdot \frac{\epsilon \Delta_A^2(S)}{\delta D}.
\end{aligned}$$

by Property 2. The lemma follows by putting the various pieces together. ∎

We can now finish off the proof of Theorem 2.

Theorem 17 *Fix any $\epsilon \le O(1/c)$. Suppose set $S \subset \mathbb{R}^D$ has the property that the top d eigenvalues of* $\mathrm{cov}(S)$ *account for more than $1 - \epsilon$ of its trace. Pick a random vector $U \sim N(0, (1/D)I_D)$ and split S into two parts,*

$$S_1 = \{x \in S : x \cdot U < s\} \;\; \textit{and} \;\; S_2 = \{x \in S : x \cdot U \ge s\},$$

where s is either $\mathrm{mean}(S \cdot U)$ *or median$(S \cdot U)$. Then with probability $\Omega(1)$, the expected average diameter shrinks by $\Omega(\Delta_A^2(S)/cd)$.*

Proof. By Lemma 7, the reduction in expected average diameter is

$$\Delta_A^2(S) - \left\{ \frac{|S_1|}{|S|} \Delta_A^2(S_1) + \frac{|S_2|}{|S|} \Delta_A^2(S_2) \right\} \;=\; \frac{2|S_1| \cdot |S_2|}{|S|^2} \|\mathrm{mean}(S_1) - \mathrm{mean}(S_2)\|^2,$$

or $2p(1-p)\|\mu_1 - \mu_2\|^2$ in the language of Lemmas 15 and 16. The rest follows from those two lemmas. ∎

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4 Appendix I: Proofs of main theorem

4.1 Proof of Lemma 8

Since U has a Gaussian distribution, and any linear combination of independent Gaussians is a Gaussian, it follows that the projection $U \cdot x$ is also Gaussian. Its mean and variance are easily seen to be zero and $\|x\|^2/D$, respectively. Therefore, writing

$$Z \;=\; \frac{\sqrt{D}}{\|x\|}\,(U \cdot x)$$

we have that $Z \sim N(0,1)$. The bounds stated in the lemma now follow from properties of the standard normal. In particular, $N(0,1)$ is roughly flat in the range $[-1,1]$ and then drops off rapidly; the two cases in the lemma statement correspond to these two regimes.

The highest density achieved by the standard normal is $1/\sqrt{2\pi}$. Thus the probability mass it assigns to the interval $[-\alpha,\alpha]$ is at most $2\alpha/\sqrt{2\pi}$; this takes care of (a). For (b), we use a standard tail bound for the normal, $\mathbb{P}(|Z| \geq \beta) \leq (2/\beta)e^{-\beta^2/2}$; see, for instance, page 7 of [7].

4.2 Proof of Lemma 9

Set $c = \sqrt{2\ln 1/(\delta\epsilon)} \geq 2$.

Fix any point x, and randomly choose a projection U. Let $\widetilde{x} = U \cdot x$ (and likewise, let $\widetilde{S} = U \cdot S$). What is the chance that $\widetilde{x}$ lands far from $\widetilde{x}_0$? Define the bad event to be $F_x = \mathbf{1}(|\widetilde{x} - \widetilde{x}_0| \geq c\Delta/\sqrt{D})$. By Lemma 8(b), we have

$$\mathbb{E}_U[F_x] \;\leq\; \mathbb{P}_U\left[|\widetilde{x} - \widetilde{x}_0| \geq c \cdot \frac{\|x - x_0\|}{\sqrt{D}}\right] \;\leq\; \frac{2}{c}\,e^{-c^2/2} \;\leq\; \delta\epsilon.$$

Since this holds for any $x \in S$, it also holds in expectation over x drawn from ν. We are interested in bounding the probability (over the choice of U) that more than an ϵ fraction of ν falls far from $\widetilde{x}_0$. Using Markov's inequality and then Fubini's theorem, we have

$$\mathbb{P}_U\left[\mathbb{E}_\mu[F_x] \geq \epsilon\right] \;\leq\; \frac{\mathbb{E}_U[\mathbb{E}_\mu[F_x]]}{\epsilon} \;=\; \frac{\mathbb{E}_\mu[\mathbb{E}_U[F_x]]}{\epsilon} \;\leq\; \delta,$$

as claimed.

4.3 Proof of Lemma 4

Let random variable X be distributed uniformly over S. Then

$$\mathbb{P}\left[\|X - \mathbb{E}X\|^2 \;\geq\; \text{median}(\|X - \mathbb{E}X\|^2)\right] \;\geq\; \frac{1}{2}$$

by definition of median, so $\mathbb{E}\left[\|X - \mathbb{E}X\|^2\right] \geq \text{median}(\|X - \mathbb{E}X\|^2)/2$. It follows from Corollary 6 that

$$\text{median}(\|X - \mathbb{E}X\|^2) \leq 2\mathbb{E}\left[\|X - \mathbb{E}X\|^2\right] = \Delta_A^2(S).$$

Set S_1 has squared diameter $\Delta^2(S_1) \leq (2\,\text{median}(\|X - \mathbb{E}X\|))^2 \leq 4\Delta_A^2(S)$. Meanwhile, S_2 has squared diameter at most $\Delta^2(S)$. Therefore,

$$\frac{|S_1|}{|S|}\Delta^2(S_1) + \frac{|S_2|}{|S|}\Delta^2(S_2) \;\leq\; \frac{1}{2}\cdot 4\Delta_A^2(S) + \frac{1}{2}\Delta^2(S)$$

and the lemma follows by using $\Delta^2(S) > c\Delta_A^2(S)$.

4.4 Proof of Lemma 12

This follows by examining the moment-generating function of $U^T AU$. Since the distribution of U is spherically symmetric, we can work in the eigenbasis of A and assume without loss of generality that $A = \text{diag}(a_1, \ldots, a_n)$, where $a_1, \ldots, a_n$ are the eigenvalues. Moreover, for convenience we take $\sum a_i = 1$.

Let $U_1, \ldots, U_n$ denote the individual coordinates of U. We can rewrite them as $U_i = Z_i/\sqrt{n}$, where $Z_1, \ldots, Z_n$ are i.i.d. standard normal random variables. Thus

$$U^T AU \;=\; \sum_i a_i U_i^2 \;=\; \frac{1}{n}\sum_i a_i Z_i^2.$$

This tells us immediately that $\mathbb{E}[U^T AU] = 1/n$.

We use Chernoff's bounding method for both parts. For (a), for any $t > 0$,

$$\begin{aligned}
\mathbb{P}\left[U^T AU < \alpha \cdot \mathbb{E}[U^T AU]\right] &= \mathbb{P}\left[\sum_i a_i Z_i^2 < \alpha\right] \;=\; \mathbb{P}\left[e^{-t\sum_i a_i Z_i^2} > e^{-t\alpha}\right] \\
&\le \frac{\mathbb{E}\left[e^{-t\sum_i a_i Z_i^2}\right]}{e^{-t\alpha}} \;=\; e^{t\alpha}\prod_i \mathbb{E}\left[e^{-ta_i Z_i^2}\right] \\
&= e^{t\alpha}\prod_i \left(\frac{1}{1+2ta_i}\right)^{1/2}
\end{aligned}$$

and the rest follows by using $t = 1/2$ along with the inequality $1/(1+x) \le e^{-x/2}$ for $0 < x \le 1$. Similarly for (b), for $0 < t < 1/2$,

$$\begin{aligned}
\mathbb{P}\left[U^T AU > \beta \cdot \mathbb{E}[U^T AU]\right] &= \mathbb{P}\left[\sum_i a_i Z_i^2 > \beta\right] \;=\; \mathbb{P}\left[e^{t\sum_i a_i Z_i^2} > e^{t\beta}\right] \\
&\le \frac{\mathbb{E}\left[e^{t\sum_i a_i Z_i^2}\right]}{e^{t\beta}} \;=\; e^{-t\beta}\prod_i \mathbb{E}\left[e^{ta_i Z_i^2}\right] \\
&= e^{-t\beta}\prod_i \left(\frac{1}{1-2ta_i}\right)^{1/2}
\end{aligned}$$

and it is adequate to choose $t = 1/4$ and invoke the inequality $1/(1-x) \le e^{2x}$ for $0 < x \le 1/2$.

4.5 Proof of Lemma 7

Let μ, μ_1, μ_2 denote the means of S, S_1, and S_2. Using Corollary 6 and Lemma 5(a), we have

$$\begin{aligned}
&\Delta_A^2(S) - \frac{|S_1|}{|S|}\Delta_A^2(S_1) - \frac{|S_2|}{|S|}\Delta_A^2(S_2) \\
&= \frac{2}{|S|}\sum_S \|x-\mu\|^2 - \frac{|S_1|}{|S|}\cdot\frac{2}{|S_1|}\sum_{S_1}\|x-\mu_1\|^2 - \frac{|S_2|}{|S|}\cdot\frac{2}{|S_2|}\sum_{S_2}\|x-\mu_2\|^2 \\
&= \frac{2}{|S|}\left\{\sum_{S_1}\left(\|x-\mu\|^2 - \|x-\mu_1\|^2\right) + \sum_{S_2}\left(\|x-\mu\|^2 - \|x-\mu_2\|^2\right)\right\} \\
&= \frac{2|S_1|}{|S|}\|\mu_1-\mu\|^2 + \frac{2|S_2|}{|S|}\|\mu_2-\mu\|^2.
\end{aligned}$$

Writing μ as a weighted average of μ_1 and μ_2 then completes the proof.

5 Appendix II: Hardness of k-means clustering

k-MEANS CLUSTERING

Input: Set of points $x_1, \ldots, x_n \in \mathbb{R}^d$; integer k.

Output: A partition of the points into clusters $C_1, \ldots, C_k$, along with a center μ_j for each cluster, so as to minimize

$$\sum_{j=1}^{k} \sum_{i \in C_j} \|x_i - \mu_j\|^2.$$

(Here $\|\cdot\|$ is Euclidean distance.) It can be checked that in any optimal solution, μ_j is the mean of the points in C_j. Thus the $\{\mu_j\}$ can be removed entirely from the formulation of the problem. From Lemma 5(b),

$$\sum_{i \in C_j} \|x_i - \mu_j\|^2 = \frac{1}{2|C_j|} \sum_{i,i' \in C_j} \|x_i - x_{i'}\|^2.$$

Therefore, the k-means cost function can equivalently be rewritten as

$$\sum_{j=1}^{k} \frac{1}{2|C_j|} \sum_{i,i' \in C_j} \|x_i - x_{i'}\|^2.$$

We consider the specific case when k is fixed to 2.

Theorem 18 *2-means clustering is an NP-hard optimization problem.*

This was recently asserted in [6], but the proof was flawed. We establish hardness by a sequence of reductions. Our starting point is a standard restriction of 3SAT that is well known to be NP-complete.

3SAT

Input: A Boolean formula in 3CNF, where each clause has exactly three literals and each variable appears at least twice.

Output: `true` if formula is satisfiable, `false` if not.

By a standard reduction from 3SAT, we show that a special case of NOT-ALL-EQUAL 3SAT is also hard. For completeness, the details are laid out in the next section.

NAESAT*

Input: A Boolean formula $\phi(x_1, \ldots, x_n)$ in 3CNF, such that (i) every clause contains exactly three literals, and (ii) each pair of variables x_i, x_j appears together in at most two clauses, once as either $\{x_i, x_j\}$ or $\{\overline{x}_i, \overline{x}_j\}$, and once as either $\{\overline{x}_i, x_j\}$ or $\{x_i, \overline{x}_j\}$.

Output: `true` if there exists an assignment in which each clause contains exactly one or two satisfied literals; `false` otherwise.

Finally, we get to a generalization of 2-MEANS.

GENERALIZED 2-MEANS

Input: An $n \times n$ matrix of interpoint distances D_{ij}.

Output: A partition of the points into two clusters C_1 and C_2, so as to minimize

$$\sum_{j=1}^{2} \frac{1}{2|C_j|} \sum_{i,i' \in C_j} D_{ii'}.$$

We reduce NAESAT* to GENERALIZED 2-MEANS. For any input ϕ to NAESAT*, we show how to efficiently produce a distance matrix $D(\phi)$ and a threshold $c(\phi)$ such that ϕ satisfies NAESAT* if and only if $D(\phi)$ admits a generalized 2-means clustering of cost $\leq c(\phi)$.

Thus GENERALIZED 2-MEANS CLUSTERING is hard. To get back to 2-MEANS (and thus establish Theorem 18), we prove that the distance matrix $D(\phi)$ can in fact be realized by squared Euclidean distances. This existential fact is also constructive, because in such cases, the embedding can be obtained in cubic time by classical multidimensional scaling [10].

5.1 Hardness of NAESAT*

Given an input $\phi(x_1, \ldots, x_n)$ to 3SAT, we first construct an intermediate formula ϕ' that is satisfiable if and only if ϕ is, and additionally has exactly three occurrences of each variable: one in a clause of size three, and two in clauses of size two. This ϕ' is then used to produce an input ϕ'' to NAESAT*.

1. Constructing ϕ'.

   Suppose variable x_i appears $k \geq 2$ times in ϕ. Create k variables $x_{i1}, \ldots, x_{ik}$ for use in ϕ': use the same clauses, but replace each occurrence of x_i by one of the x_{ij}. To enforce agreement between the different copies x_{ij}, add k additional clauses $(\overline{x}_{i1} \vee x_{i2}), (\overline{x}_{i2} \vee x_{i3}), \ldots, (\overline{x}_{ik}, x_{i1})$. These correspond to the implications $x_1 \Rightarrow x_2, x_2 \Rightarrow x_3, \ldots, x_k \Rightarrow x_1$.

   By design, ϕ is satisfiable if and only if ϕ' is satisfiable.

2. Constructing ϕ''.

   Now we construct an input ϕ'' for NAESAT*. Suppose ϕ' has m clauses with three literals and m' clauses with two literals. Create $2m + m' + 1$ new variables: $s_1, \ldots, s_m$ and $f_1, \ldots, f_{m+m'}$ and f.

   If the jth three-literal clause in ϕ' is $(\alpha \vee \beta \vee \gamma)$, replace it with two clauses in ϕ'': $(\alpha \vee \beta \vee s_j)$ and $(\overline{s}_j \vee \gamma \vee f_j)$. If the jth two-literal clause in ϕ' is $(\alpha \vee \beta)$, replace it with $(\alpha \vee \beta \vee f_{m+j})$ in ϕ''. Finally, add $m + m'$ clauses that enforce agreement among the f_i: $(\overline{f}_1 \vee f_2 \vee f), (\overline{f}_2 \vee f_3 \vee f), \ldots, (\overline{f}_{m+m'} \vee f_1 \vee f)$.

   All clauses in ϕ'' have exactly three literals. Moreover, the only pairs of variables that occur together (in clauses) more than once are $\{f_i, f\}$ pairs. Each such pair occurs twice, as $\{f_i, f\}$ and $\{\overline{f}_i, f\}$.

Lemma 19 *ϕ' is satisfiable if and only if ϕ'' is not-all-equal satisfiable.*

Proof. First suppose that ϕ' is satisfiable. Use the same settings of the variables for ϕ''. Set $f = f_1 = \cdots = f_{m+m'} =$ `false`. For the jth three-literal clause $(\alpha \vee \beta \vee \gamma)$ of ϕ', if $\alpha = \beta =$ `false` then set s_j to `true`, otherwise set s_j to `false`. The resulting assignment satisfies exactly one or two literals of each clause in ϕ''.

Conversely, suppose ϕ'' is not-all-equal satisfiable. Without loss of generality, the satisfying assignment has f set to `false` (otherwise flip all assignments). The clauses of the form $(\overline{f}_i \vee f_{i+1} \vee f)$ then enforce agreement among all the f_i variables. We can assume they are all `false` (otherwise, once again, flip all assignments). This means the two-literal clauses of ϕ' must be satisfied. Finally, consider any three-literal clause $(\alpha \vee \beta \vee \gamma)$ of ϕ'. This was replaced by $(\alpha \vee \beta \vee s_j)$ and $(\overline{s}_j \vee \gamma \vee f_j)$ in ϕ''. Since f_j is `false`, it follows that one of the literals α, β, γ must be satisfied. Thus ϕ' is satisfied. ∎

5.2 Hardness of GENERALIZED 2-MEANS

Given an instance $\phi(x_1, \ldots, x_n)$ of NAESAT*, we construct a $2n \times 2n$ distance matrix $D = D(\phi)$ where the (implicit) $2n$ points correspond to literals. Entries of this matrix will be indexed as $D_{\alpha,\beta}$, for $\alpha, \beta \in \{x_1, \ldots, x_n, \overline{x}_1, \ldots, \overline{x}_n\}$. Another bit of notation: we write $\alpha \sim \beta$ to mean that either α and β occur together in a clause or $\overline{\alpha}$ and $\overline{\beta}$ occur together in a clause. For instance, the clause $(x \vee \overline{y} \vee z)$ allows one to assert $\overline{x} \sim y$ but not $x \sim y$. The input restrictions on NAESAT* ensure that every relationship $\alpha \sim \beta$ is generated by a unique clause; it is not possible to have two different clauses that both contain either $\{\alpha, \beta\}$ or $\{\overline{\alpha}, \overline{\beta}\}$.

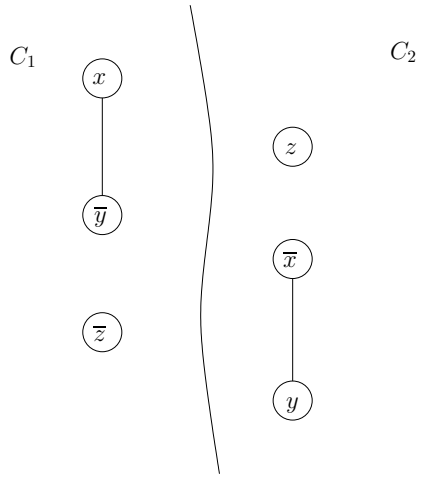
Define

$$D_{\alpha,\beta} = \begin{cases} 0 & \text{if } \alpha = \beta \\ 1+\Delta & \text{if } \alpha = \overline{\beta} \\ 1+\delta & \text{if } \alpha \sim \beta \\ 1 & \text{otherwise} \end{cases}$$

Here $0 < \delta < \Delta < 1$ are constants such that $4\delta m < \Delta \leq 1 - 2\delta n$, where m is the number of clauses of ϕ. One valid setting is $\delta = 1/(5m + 2n)$ and $\Delta = 5\delta m$.

Lemma 20 *If ϕ is a satisfiable instance of* NAESAT*, *then $D(\phi)$ admits a generalized 2-means clustering of cost $c(\phi) = n - 1 + 2\delta m/n$, where m is the number of clauses of ϕ.*

Proof. The obvious clustering is to make one cluster (say C_1) consist of the positive literals in the satisfying not-all-equal assignment and the other cluster (C_2) the negative literals. Each cluster has n points, and the distance between any two distinct points α, β within a cluster is either 1 or, if $\alpha \sim \beta$, $1 + \delta$. Each clause of ϕ has at least one literal in C_1 and at least one literal in C_2, since it is a not-all-equal assignment. Hence it contributes exactly one $\sim$ pair to C_1 and one $\sim$ pair to C_2. The figure below shows an example with a clause $(x \vee \overline{y} \vee z)$ and assignment $x = \texttt{true}, y = z = \texttt{false}$.



Thus the clustering cost is

$$\begin{aligned} \frac{1}{2n}\sum_{i,i' \in C_1} D_{ii'} + \frac{1}{2n}\sum_{i,i' \in C_2} D_{ii'} &= 2 \cdot \frac{1}{n}\left(\binom{n}{2} + m\delta\right) \\ &= n - 1 + \frac{2\delta m}{n}. \end{aligned}$$

∎

Lemma 21 *Let C_1, C_2 be any 2-clustering of $D(\phi)$. If C_1 contains both a variable and its negation, then the cost of this clustering is at least $n - 1 + \Delta/(2n) > c(\phi)$.*

Proof. Suppose C_1 has n' points while C_2 has $2n - n'$ points. Since all distances are at least 1, and since C_1 contains a pair of points at distance $1 + \Delta$, the total clustering cost is at least

$$\frac{1}{n'}\left(\binom{n'}{2} + \Delta\right) + \frac{1}{2n - n'}\binom{2n - n'}{2} = n - 1 + \frac{\Delta}{n'} \geq n - 1 + \frac{\Delta}{2n}.$$

Since $\Delta > 4\delta m$, this is always more than $c(\phi)$. ∎

Lemma 22 *If $D(\phi)$ admits a 2-clustering of cost $\leq c(\phi)$, then ϕ is a satisfiable instance of* NAESAT*.

Proof. Let C_1, C_2 be a 2-clustering of cost $\leq c(\phi)$. By the previous lemma, neither C_1 nor C_2 contain both a variable and its negation. Thus $|C_1| = |C_2| = n$. The cost of the clustering can be written as

$$\frac{2}{n}\left(\binom{n}{2} + \delta \sum_{\text{clauses}} \left\{ \begin{array}{ll} 1 & \text{if clause split between } C_1, C_2 \\ 3 & \text{otherwise} \end{array} \right\}\right)$$

Since the cost is $\leq c(\phi)$, it follows that *all* clauses are split between C_1 and C_2, that is, every clause has at least one literal in C_1 and one literal in C_2. Therefore, the assignment that sets all of C_1 to `true` and all of C_2 to `false` is a valid NAESAT* assignment for ϕ. ∎

5.3 Embeddability of $D(\phi)$

We now show that $D(\phi)$ can be embedded into l_2^2, in the sense that there exist points $x_\alpha \in \mathbb{R}^{2n}$ such that $D_{\alpha,\beta} = \|x_\alpha - x_\beta\|^2$ for all α, β. We rely upon the following classical result [17].

Theorem 23 (Schoenberg) *Let H denote the matrix $I - (1/N)\mathbf{1}\mathbf{1}^T$. An $N \times N$ symmetric matrix D can be embedded into l_2^2 if and only if $-HDH$ is positive semidefinite.*

The following corollary is immediate.

Corollary 24 *An $N \times N$ symmetric matrix D can be embedded into l_2^2 if and only if $u^T D u \leq 0$ for all $u \in \mathbb{R}^N$ with $u \cdot \mathbf{1} = 0$.*

Proof. Since the range of the map $v \mapsto Hv$ is precisely $\{u \in \mathbb{R}^N : u \cdot \mathbf{1} = 0\}$, we have

$$\begin{array}{rcl} -HDH \text{ is positive semidefinite} & \Leftrightarrow & v^T HDHv \leq 0 \text{ for all } v \in \mathbb{R}^N \\ & \Leftrightarrow & u^T Du \leq 0 \text{ for all } u \in \mathbb{R}^N \text{ with } u \cdot \mathbf{1} = 0. \end{array}$$

∎

Lemma 25 *$D(\phi)$ can be embedded into l_2^2.*

Proof. If ϕ is a formula with variables $x_1, \ldots, x_n$, then $D = D(\phi)$ is a $2n \times 2n$ matrix whose first n rows/columns correspond to $x_1, \ldots, x_n$ and remaining rows/columns correspond to $\overline{x}_1, \ldots, \overline{x}_n$. The entry for literals (α, β) is

$$D_{\alpha\beta} = 1 - \mathbf{1}(\alpha = \beta) + \Delta \cdot \mathbf{1}(\alpha = \overline{\beta}) + \delta \cdot \mathbf{1}(\alpha \sim \beta),$$

where $\mathbf{1}(\cdot)$ denotes the indicator function.

Now, pick any $u \in \mathbb{R}^{2n}$ with $u \cdot \mathbf{1} = 0$. Let u^+ denote the first n coordinates of u and u^- the last n coordinates.

$$\begin{array}{rcl} u^T Du & = & \displaystyle\sum_{\alpha,\beta} D_{\alpha\beta} u_\alpha u_\beta \\ & = & \displaystyle\sum_{\alpha,\beta} u_\alpha u_\beta \left(1 - \mathbf{1}(\alpha = \beta) + \Delta \cdot \mathbf{1}(\alpha = \overline{\beta}) + \delta \cdot \mathbf{1}(\alpha \sim \beta)\right) \\ & = & \displaystyle\sum_{\alpha,\beta} u_\alpha u_\beta - \sum_\alpha u_\alpha^2 + \Delta \sum_\alpha u_\alpha u_{\overline{\alpha}} + \delta \sum_{\alpha,\beta} u_\alpha u_\beta \mathbf{1}(\alpha \sim \beta) \\ & \leq & \displaystyle\left(\sum_\alpha u_\alpha\right)^2 - \|u\|^2 + 2\Delta(u^+ \cdot u^-) + \delta \sum_{\alpha,\beta} |u_\alpha||u_\beta| \\ & \leq & \displaystyle -\|u\|^2 + \Delta(\|u^+\|^2 + \|u^-\|^2) + \delta \left(\sum_\alpha |u_\alpha|\right)^2 \\ & \leq & -(1-\Delta)\|u\|^2 + 2\delta\|u\|^2 n \end{array}$$

where the last step uses the Cauchy-Schwarz inequality. Since $2\delta n \leq 1 - \Delta$, this quantity is always ≤ 0. ∎